Locally Exact Lower Bounds and Optimality Cuts for All-Quadratic Programs with Convex Constraints

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Abstract

A central problem of branch-and-bound methods for global optimization is that lower bounds are often not exact even if the diameter of the subdivided regions shrinks to zero. This can lead to a large number of subdivisions preventing the method from terminating in reasonable time. For the all-quadratic optimization problem with convex constraints we present locally exact lower bounds and optimality cuts based on Lagrangian relaxation. If all global minimizers fulfill a certain second order optimality condition it can be shown that locally exact lower bounds or optimality cuts lead to finite termination of a branch-and-bound algorithm. Since there exist efficient methods for computing Lagrangian relaxation bounds of all-quadratic optimization problems exploiting problem structure our approach should be applicable to large scale structured optimization problems.

Keywords: global optimization, nonconvex quadratic programming, Lagrangian relaxation, locally exact lower bounds, optimality cuts

AMS subject classification: 90C20, 90C30, 90C06, 65K05

1 Introduction

In this paper we consider the following all-quadratic optimization problem:

$$
\text{(Q)} \qquad \begin{array}{ll} \text{global minimize} & q_0(x) \\ \text{subject to} & q_i(x) \le 0, \quad i \in I_{in} \\ & q_i(x) = 0, \quad i \in I_{eq} \end{array}
$$

where $q_i(x) := \frac{1}{2}x^T A_i x + b_i^T x + c_i$, $A_i \in I\!R^{(n,n)}, b_i \in I\!R^n, c_i \in I\!R$, $i \in I_{in} \cup I_{eq} \cup \{0\}$. It is assumed that the constraints of problem (Q) are convex. Note that this convexity assumption implies that the equality constraints are linear.

Problem (Q) plays an interesting role in global optimization. Important special cases of (Q) are for example the trust region problem with one or several ellipsoid constraints, the box-constrained quadratic program and the standard quadratic program. It is known that problem (Q) is NP-hard [12]. For applications and solution methods we refer to [8, 2, 6, 13, 25, 18, 19, 21, 3, 4, 20]. Many solution methods for problem (Q) are based on the branch-and-bound (B&B) principle. A well-known difficulty of B&B algorithms is that often regions containing a global minimizer have to be subdivided very often in order to get almost exact lower bounds. In large dimensions this can prevent the method from terminating in reasonable time. Almost all existing bounding methods for problem (Q) produce lower bounds which are usually not exact. This can lead to infinitely many iterations of a B&B algorithm. Finite termination of B&B algorithms can be proved often only for so-called ϵ-optimal solutions. We propose two methods for avoiding this difficulty:

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- locally exact lower bounds
- optimality cuts.

Locally exact lower bounds are lower bounds which are exact if the partition sets are sufficiently small. An optimality cut is a cutting plane which cuts off a part of the feasible set containing a solution point. An important property of locally exact lower bounds and optimality cuts is that under certain assumptions they lead to finite termination of a B&B procedure. To our knowledge, only the linear programming bound presented in [7] is a locally exact lower bound for (Q).

The paper is organized as follows. In §2 we describe two B&B algorithms for solving problem (Q) in finite time using either locally exact lower bounds or optimality cuts. In §3 we give some results on Lagrangian relaxation bounds for problem (Q) and discuss in §4 how these bounds can be improved. Using these results we show in §5 how locally exact lower bounds can be obtained. Optimality cuts are derived in §6 applying previous results. We finish with some conclusions.

2 Finite Branch-and-Bound Algorithms

In this section we describe two B&B algorithms for solving problem (Q) in finitely many iterations. We begin with the description of basic operations of a B&B algorithm.

2.1 Basic B&B Operations

Partition Sets

Denote by $\Omega \subset I\!R^n$ the feasible set of problem (Q). Let $S_1, .., S_r$ be subsets of $I\!R^n$ such that

$$\bigcup_{i=1}^{r} S_i \supset \Omega \quad \text{and} \quad \text{int } S_i \cap \text{ int } S_j = \emptyset \text{ for } i \neq j.$$

Each subset S_i is called partition set and the collection of partition sets denoted by $\mathcal{P} := \{S_1, .., S_r\}$ is called a partition of Ω.

Subdivision Methods

A subdivision method defines from a given partition a new partition by subdividing one are several partition sets. A nested subsequence of partition sets $\{S_i\}$, (i.e. $S_{i+1} \subset S_i \quad \forall i$), is called exhaustive if S_i shrinks to a unique point, i.e. $\bigcap_{i=1}^{\infty} S_i = \{x\}$. A partition method is called exhaustive if every nested subsequence of partition sets generated by the subdivision method is exhaustive. Examples for exhaustive partition methods are given in [12].

Lower Bounds

The optimal value of $q_0(x)$ over $\Omega \cap S$ is denoted by

$$q^*(S) := \begin{cases} \min\limits_{x \in \Omega \cap S} q_0(x) & : \quad \text{if } \Omega \cap S \neq \emptyset \\ \infty & : \quad \text{else} \end{cases} . \tag{1}$$

A lower bound of $q^*(S)$ is denoted by $\mu(S)$. A lower bound is called **tight** if

$$\lim_{i \to \infty} \mu(S_i) = \begin{cases} q_0(\hat{x}) & : \quad \text{if } \hat{x} \in \Omega \\ \infty & : \quad \text{else} \end{cases}$$

where $\{S_i\}$ is an exhaustive nested subsequence with $\bigcap_{i=1}^{\infty} S_i = \{\hat{x}\}$. A lower bound $\mu(S)$ is called **locally exact** with respect to a local minimizer x^* of problem (Q) if there exist $\delta > 0$ such that $q^*(S) = q_0(x^*) = \mu(S)$ for all S with $x^* \in S$ and $\operatorname{diam} S \leq \delta$. Note that this implies that for an exhaustive nested subsequence $\{S_i\}$ with $\bigcap_{i=1}^{\infty} S_i = \{x^*\}$ there exist $N \in \mathbb{N}$ such that $q^*(S_i) = \mu(S_i)$ for $i \geq N$.

Upper Bounds

Let $F(S) \in \mathbb{R}^n$ be an estimate of a global minimizer of q_0 over $\Omega \cap S$ with the property: $F(S)$ is a local minimizer of q_0 over $\Omega \cap S$ for all S with $S \cap \Omega \neq \emptyset$ if $\operatorname{diam}(S)$ is sufficiently small. If a feasible point is available this can be achieved by a local search method starting from the feasible point. Otherwise a projection should be defined which provides a feasible point if the distance from a given unfeasible point to the feasible set is small enough. An upper bound of $q^*(S)$ is defined by

$$\gamma(S) := \begin{cases} q_0(F(S)) & : \quad \text{if } F(S) \in \Omega \\ \infty & : \quad \text{else} \end{cases}$$

Optimality Cuts

Given a local minimizer $x^* \in \Omega$ of problem (Q) we call a halfspace $H := \{x \in \mathbb{R}^n : \eta^T x \leq \gamma\}$ where $\eta \in \mathbb{R}^n$ and $\gamma \in \mathbb{R}$ an optimality cut if $x^* \in \operatorname{int} H$ and $q^*(H) = q_0(x^*)$.

2.2 Branch-and-Bound using Locally Exact Lower Bounds

We describe now a B&B algorithm for solving problem (Q) which uses two different bounding methods denoted by $\mu_1(S)$ and $\mu_2(S)$ respectively. We denote by q_{opt} the actual estimate of the optimal value.

Algorithm 1

1 *determine* $S \subset \mathbb{R}^n$ *such that* $S \supset \Omega$, *set* $\mu(S) = \mu_1(S)$, *set* $\mathcal{P} = \{S\}$ *and* $q_{opt} = +\infty$;
2 **repeat**
3   *choose* $\hat{S} \in \mathcal{P}$ *such that* $\mu(\hat{S}) = \min_{S \in \mathcal{P}} \mu(S)$ *and set* $\mathcal{P} = \mathcal{P} \setminus \{\hat{S}\}$;
4   *compute* $F(\hat{S})$;
5   **if** $\gamma(\hat{S}) \leq q_{opt}$ *and* $\gamma(\hat{S}) \neq \infty$
6   *set* $q_{opt} = \gamma(\hat{S})$.
7   *try to compute a locally exact lower bound* $\mu_2(\hat{S})$ *with respect to* $F(\hat{S})$;
8   **if** *this is possible and* $\mu_2(\hat{S}) = q^*(\hat{S})$ **goto** *11*
9   **endif**
10   *subdivide* $\hat{S}$ *into* $S_1, .., S_p$, *set* $\mu(S) = \mu_1(S_1), .., \mu(S) = \mu_1(S_p)$ *and* $\mathcal{P} = \mathcal{P} \cup \{S_1, .., S_p\}$;
11   *delete elements* $S \in \mathcal{P}$ *with* $\mu(S) \geq q_{opt}$.
12 **until** $\mathcal{P} = \emptyset$.

Proposition 1 *Assume that $\Omega \neq \emptyset$, the lower bounding method $\mu_1(S)$ is tight and the subdivision method of Algorithm 1 is exhaustive. Assume further that it is possible to compute a locally exact lower bound $\mu_2(S)$ with respect to $\hat{x}$ if $\hat{x}$ is a global minimizer of problem (Q). Then Algorithm 1 terminates after finitely many iterations.*

Proof. Assume that Algorithm 1 does not terminate in finite time. Then there exist a nested subsequence of partition elements $\{S_i\}$ generated by Algorithm 1 such that $\mu(S_i)$ is the global lower bound of the corresponding partition, i.e. $\mu(S_i) = \min_{S \in \mathcal{P}_i} \mu(S)$, implying $\mu(S_i) \leq q^*$. Since the partition method is exhaustive we have $\bigcap_{i=1}^{\infty} S_i = \{\hat{x}\}$. We show now that the sequence $\{S_i\}$ is finite which proves the assertion. If $\hat{x}$ is a global minimizer of (Q) we have $F(S_i) = \hat{x}$ for $i \geq N$ and N sufficiently large. Since in this case $\mu(S_i) = \mu_2(S_i)$ the sequence must be finite due to the local exactness of $\mu_2(S_i)$ with respect to $\hat{x}$. If $\hat{x}$ is not a global minimizer then either $\hat{x} \notin \Omega$, implying $\mu(S_i) \to \infty$, or $\hat{x} \in \Omega$ and $q_0(\hat{x}) > q^*$, implying $\mu(S_i) \to q_0(\hat{x})$ since $\mu(S_i)$ is tight. In both cases it follows $\mu(S_i) > q^*$ if i is sufficiently large. This contradicts $\mu(S_i) \leq q^*$.

□

Note that lower bounds applied to integer programs are usually locally exact implying that corresponding B&B algorithms are finite.

2.3 Branch-and-Bound using Optimality Cuts

Instead of using locally exact lower bounds it is often more efficient to use optimality cuts. The following B&B algorithm solves problem (Q) in finite time using optimality cuts and tight lower bounds. We use the same notation as above.

Algorithm 2

1 *determine* $S \subset \mathbb{R}^n$ *such that* $S \supset \Omega$, *compute* $\mu(S)$, *set* $\mathcal{P} = \{S\}$ *and* $q_{opt} = +\infty$;
2 **repeat**
3 *choose* $\hat{S} \in \mathcal{P}$ *such that* $\mu(\hat{S}) = \min_{S \in \mathcal{P}} \mu(S)$ *and set* $\mathcal{P} = \mathcal{P} \setminus \{\hat{S}\}$;
4 *compute* $F(\hat{S})$;
5 **if** $\gamma(\hat{S}) \leq q_{opt}$ *and* $\gamma(\hat{S}) \neq \infty$
6 *set* $q_{opt} = \gamma(\hat{S})$;
7 *try to compute an optimality cut* H *with respect to* $F(\hat{S})$;
8 **if** *this is possible : compute* $\mu(\hat{S} \setminus H)$, *set* $\mathcal{P} = \mathcal{P} \cup \{\hat{S} \setminus H\}$ *and* **goto** *11*
9 **endif**
10 *subdivide* $\hat{S}$ *into* $S_1, .., S_p$, *compute* $\mu(S_1), .., \mu(S_p)$ *and set* $\mathcal{P} = \mathcal{P} \cup \{S_1, .., S_p\}$;
11 *delete elements* $S \in \mathcal{P}$ *with* $\mu(S) \geq q_{opt}$.
12 **until** $\mathcal{P} = \emptyset$.

Proposition 2 *Assume that $\Omega \neq \emptyset$, the lower bounding method $\mu(S)$ is tight and the subdivision method of Algorithm 2 is exhaustive. Assume further that it is possible to make an optimality cut with respect to $\hat{x}$ if $\hat{x}$ is a global minimizer of problem (Q). Then Algorithm 2 terminates after finitely many iterations.*

Proof. Assume that Algorithm 2 does not terminate in finite time. Then there exist a sequence $\{S_i\}$ as defined in Proposition 1 shrinking to $\{\hat{x}\}$. If $\hat{x}$ is a global minimizer of (Q) there exist $N \in \mathbb{N}$ such that $F(S_N) = \hat{x}$. In this case the algorithm makes an optimality cut of S_N with respect to $\hat{x}$ proving the finiteness of $\{S_i\}$. The remainder of the proof is equal to the proof of Proposition 1.

□

3 Lagrangian Relaxation

We describe now the method for obtaining lower bounds for problem (Q) based on Lagrangian relaxation.

3.1 Basic Principle

The Lagrange function of problem (Q) is the quadratic form

$$L(x,\alpha) := q_0(x) + \sum_{i\in I} \alpha_i q_i(x),$$

where $I := I_{in} \cup I_{eq}$. Consider the Lagrange problem

$$\Psi(\alpha) := \min_{x\in \mathbb{R}^n} L(x,\alpha). \tag{2}$$

The dual bound is defined by

$$\Psi^* := \max_{\alpha\in \mathbb{R}^I} \quad \Psi(\alpha) \qquad \text{subject to} \quad \alpha_i \geq 0, \quad i \in I_{in}. \tag{3}$$

By weak duality we have

$$q^* - \Psi^* \geq 0.$$

The quantity $q^* - \Psi^*$ is called duality gap. It is well-known that due to the nonconvexity of problem (Q) it is possible that a nonzero duality gap can occur. However, if (Q) is convex and satisfies a Slater condition then $q^* - \Psi^* = 0$. Note that most of the existing lower bounding methods do not have this useful property.

3.2 Equivalent Formulations of the Dual Bound

Interestingly (3) can be formulated as a semidefinite program (SDP). We use the notation $A \succeq 0$ for a matrix A to be positive semidefinite.

Lemma 1 *Let $\hat{x} \in \mathbb{R}^n$ be an arbitrary point, $Q(\alpha, y) \in \mathbb{R}^{(n+1,n+1)}$ the matrix defined by*

$$Q(\alpha,y) := \begin{pmatrix} \frac{1}{2}\nabla_x^2 L(\hat{x},\alpha) & \frac{1}{2}\nabla_x L(\hat{x},\alpha) \\ \frac{1}{2}\nabla_x L(\hat{x},\alpha)^T & L(\hat{x},\alpha) - y \end{pmatrix}$$

and $\mathcal{S} \subset \mathbb{R}^I \times \mathbb{R}$ the set defined by

$$\mathcal{S} := \{(\alpha, y) \in \mathbb{R}^I \times \mathbb{R} : Q(\alpha,y) \succeq 0, \alpha_i \geq 0, i \in I_{in}\}. \tag{4}$$

Then

$$\Psi^* = \max_{(\alpha,y)\in\mathcal{S}} y. \tag{5}$$

Proof. Let $(\hat{\alpha}, \hat{y})$ be a solution of (5). Since $Q(\hat{\alpha},\hat{y}) \succeq 0$ we have

$$\begin{aligned}
&\begin{pmatrix} x-\hat{x} \\ 1 \end{pmatrix}^T Q(\hat{\alpha},\hat{y}) \begin{pmatrix} x-\hat{x} \\ 1 \end{pmatrix} \\
&= \frac{1}{2}(x-\hat{x})^T \nabla_x^2 L(\hat{x},\hat{\alpha})(x-\hat{x}) + \nabla_x L(\hat{x},\hat{\alpha})^T(x-\hat{x}) + L(\hat{x},\hat{\alpha}) - \hat{y} \\
&= L(x,\hat{\alpha}) - \hat{y} \geq 0 \quad \forall x \in \mathbb{R}^n.
\end{aligned}$$

This implies $\hat{y} \leq \min_{x\in I\!R^n} L(x,\hat{\alpha}) \leq \Psi^*$. Now let (α^*, x^*) be a solution of (3), i.e. $\Psi^* = L(x^*, \alpha^*)$. If $\Psi^* = -\infty$ we have obviously $\Psi^* \leq \hat{y}$. If $\Psi^* > -\infty$ it follows $\nabla_x^2 L(x,\alpha^*) \succeq 0$ and $\nabla L(x^*, \alpha^*) = 0$ implying $Q(\alpha^*, \Psi^*) = \begin{pmatrix} \frac{1}{2}\nabla_x^2 L(x^*,\alpha^*) & 0 \\ 0 & 0 \end{pmatrix} \succeq 0$. Therefore, $(\alpha^*, \Psi^*) \in \mathcal{S}$ and hence $\Psi^* \leq \hat{y}$. □

The next Lemma gives a further equivalent formulation of Ψ^*.

Lemma 2 *Let $I_{lin} \subset I$ and $I_q \subset I$ be the index sets of linear constraints and quadratic constraints of problem (Q) respectively. Define the Lagrangian with respect to quadratic constraints*

$$L_q(x,\alpha) := q_0(x) + \sum_{i\in I_q} \alpha_i q_i(x)$$

and the feasible set with respect to linear constraints

$$P := \{x \in I\!R^n : q_i(x) \leq 0, i \in I_{in} \cap I_{lin}, q_j(x) = 0, j \in I_{eq} \cap I_{lin}\}.$$

If $\Psi^* > -\infty$ then

$$\Psi^* = \max\{\min_{x\in P} L_q(x,\alpha) : \alpha_i \geq 0, i \in I_{in} \cap I_q, \nabla_x^2 L_q(x,\alpha) \succeq 0\}. \tag{6}$$

Proof. Let $\alpha^* = (\alpha_q^*, \alpha_l^*)$ be a solution of (3) where α_q^* corresponds to quadratic constraints and α_l^* corresponds to linear constraints of (Q). From $\Psi^* > -\infty$ it follows $\nabla_x^2 L(x,\alpha^*) = \nabla_x^2 L_q(x,\alpha_q^*) \succeq 0$. It holds

$$\begin{aligned} \Psi^* &= \{\max \Psi(\alpha) : \alpha_i \geq 0, i \in I_{in}\} \\ &= \{\max \Psi(\alpha_q^*, \alpha_l) : \alpha_i \geq 0, i \in I_{in} \cap I_{lin}\} \\ &= \{\max \min_{x\in I\!R^n} L(x, \alpha_q^*, \alpha_l) : \alpha_i \geq 0, i \in I_{in} \cap I_{lin}\} \\ &= \min_{x\in P} L_q(x,\alpha_q^*) \leq \Psi_q^* \end{aligned}$$

where Ψ_q^* is the optimal value of the right-hand side of (6). The last equation follows from strong duality since $L_q(x,\alpha_q^*)$ is convex (see [12]). On the other hand we have

$$\begin{aligned} \Psi_q^* &= \max\{\min_{x\in P} L_q(x,\alpha_q) : \alpha_i \geq 0, i \in I_{in} \cap I_q, \nabla_x^2 L_q(x,\alpha_q) \succeq 0\} \\ &= \max\{\min_{x\in I\!R^n} L(x,\alpha) : \alpha_i \geq 0, i \in I_{in}, \nabla_x^2 L(x,\alpha) \succeq 0\} \leq \Psi^*. \end{aligned}$$

The last equation follows from strong duality since $L_q(x,\alpha_q)$ is convex. This proves $\Psi^* = \Psi_q^*$. □

Note that by including quadratic box constraints $(\underline{x}_i - x_i)(\bar{x}_i - x_i) \leq 0$, $1 \leq i \leq n$ into (Q) it can be shown that $\Psi^* > -\infty$.

3.3 Computing Ψ^*

In the last years many methods for computing Ψ^* have been proposed. These methods can be divided into three classes. The first class are methods for solving a semidefinite program similar as (5), see for example [9] for solution methods and applications of semidefinite programming. Most of these algorithms are interior point methods which usually converge fast if the size of the problem is moderate. However, for large scale problems the convegence can be slow if it is not possible to exploit problem structure. The second class are methods based on eigenvalue optimization. In [11] the Lagrangian relaxation bound for the max-cut problem is computed by formulating (3) as an eigenvalue optimization problem and solving this problem by the so-called spectral bundle method. In [11, 10] numerical results for large scale structured problems are presented indicating that this bundle method is faster than an interior point method. A third approach for computing Ψ^* is proposed by Shor [24]. This approach is based on maximizing an exact penalty function over $\mathbb{R}^I$. Numerical results on this approach using the so-called r-algorithm for maximizing a nonsmooth penalty function are reported in [24]. An advantage of using nonsmooth optimization methods for is that they often can exploit problem structure making them attractive for large scale structured optimization problems.

4 Improving Dual Bounds

Several methods for improving dual bounds are known (see [15]). One of the most promising method is to add redundant constraints to the original problem. We explain this approach in the following.

4.1 Adding Redundant Constraints

Shor proposed in [22, 23, 24] a method for improving the Lagrangian relaxation bound by introducing redundant constraints. Let $q_i(x), i \in \hat{I}_{in} \setminus I_{in} \cup \hat{I}_{eq} \setminus I_{eq}$ be quadratic forms such that $q_i(x) \le 0$ for $i \in \hat{I}_{in} \setminus I_{in}$ and $q_i(x) = 0$ for $i \in \hat{I}_{eq} \setminus I_{eq}$ for all $x \in \Omega$ where $\hat{I}_{in} \supset I_{in}$ and $\hat{I}_{eq} \supset I_{eq}$. Consider the following extended all-quadratic program:

$$
\text{(QE)} \qquad \begin{array}{rll} \text{global minimize} & q_0(x) & \\ \text{subject to} & q_i(x) \le 0, & i \in \hat{I}_{in} \\ & q_i(x) = 0, & i \in \hat{I}_{eq} \end{array}
$$

Lemma 3 *Denote by q_e^* and by Ψ_e^* the optimal value and the dual bound of (QE) respectively. It holds*

$$\Psi^* \le \Psi_e^* \le q^* = q_e^*.$$

Proof. Since Ω is not changed by the redundant constraints we have $q_e^* = q^*$. Denote by Ψ_e the Lagrange function of problem (QE). Since $\operatorname{dom} \Psi \subset \operatorname{dom} \Psi_e$ it follows $\Psi^* \le \Psi_e^*$.

□

4.2 Closing the Duality Gap

We discuss now if the duality gap of problem (QE) can be closed by adding redundant constraints. The duality gap of problem (QE) is studied in [5] for special cases. If problem (QE) is convex satisfying a Slater condition there is no duality gap. Also for the trust region problem with one ellipsoid constraint it is known that the duality gap is zero. However, in the presence of two ellipsoid constraints a nonzero duality gap can occur. Shor proved in [23] that problem (QE) has a nonzero duality gap if and only if the objective function of an equivalent unconstrained polynomial programming problem can be represented as a sum of squares of other polynomials. However, in practice it is not known in general how to compute the polynomials. The following simple result gives a theoretical answer to the question if it is possible to close the duality gap of problem (QE) by adding a single quadratic constraint.

Lemma 4 *Assume that the inequality constraint $q^* - q_0(x) \le 0$ is included in problem (QE). Then $\Psi_e^* = q^*$.*

Proof. Choosing the Lagrange parameter corresponding to the inequality constraint $q^* - q_0(x) \leq 0$ equal to one and setting the remaining Lagrange parameters zero gives $L_e(x, \alpha) = q^*$ implying $\Psi_e^* \geq q^*$. Since $\Psi_e^* \leq q^*$ the statement is proved.

□

Of course, Lemma 4 is not very useful in practice since the optimal value q^* is not known in advance. The following global optimality criterion provides a more constructive condition.

Lemma 5
Let $\hat{I} := \hat{I}_{in} \cup \hat{I}_{eq}$. It holds $\Psi_e^* = q^*$ if and only if there exist $\hat{\alpha} \in I\!R^{\hat{I}}$ and $\hat{x} \in \Omega$ such that

$$\hat{\alpha}_i \geq 0 \text{ for all } i \in \hat{I}_{in}, \qquad L_e(\hat{x}, \hat{\alpha}) = q_0(\hat{x}), \quad \nabla_x L_e(\hat{x}, \hat{\alpha}) = 0 \text{ and } \nabla_x^2 L_e(\hat{x}, \hat{\alpha}) \succeq 0. \tag{7}$$

Proof.
Let (α^*, q^*) be a solution of (5) and x^* be a global minimizer of problem (Q). From (5) we have

$$\begin{pmatrix} \frac{1}{2}\nabla_x^2 L_e(x^*, \alpha^*) & \frac{1}{2}\nabla_x L_e(x^*, \alpha^*) \\ \frac{1}{2}\nabla_x L_e(x^*, \alpha^*)^T & L_e(x^*, \alpha^*) - \Psi_e^* \end{pmatrix} \succeq 0. \tag{8}$$

Therefore, $L_e(x^*, \alpha^*) - \Psi_e^* \geq 0$ and hence

$$\Psi_e^* \leq L_e(x^*, \alpha^*) \leq q_0(x^*) = \Psi_e^*$$

yielding $L_e(x^*, \alpha^*) = q_0(x^*)$. From (8) it follows $\nabla_x L_e(x^*, \alpha^*) = 0$ and $\nabla_x^2 L_e(x^*, \alpha^*) \succeq 0$.

Now let $(\hat{\alpha}, \hat{x})$ be a point satisfying (7). Since $Q(\hat{\alpha}, q_0(\hat{x})) \succeq 0$ we have $(\hat{\alpha}, q_0(\hat{x})) \in \mathcal{S}$ implying $\Psi_e^* \geq q_0(\hat{x})$ (see (5)). Using $\Psi_e^* \leq q_0(\hat{x})$ we obtain $\Psi_e^* = q_0(\hat{x})$.

□

5 Locally Exact Lower Bounds

Using the previous results we describe now a method for constructing locally exact lower bounds for problem (Q) based on Lagrangian relaxation.

5.1 Notation

Let $S \subset I\!R^n$ be a partition set such that $\Omega \cap S \neq \emptyset$. We assume in the sequel that S is a polytope defined by some linear inequalities. The extended quadratic program with respect to a partition set S reads

$$\text{(QE(S))} \qquad \begin{array}{rll} \text{global minimize} & q_0(x) & \\ \text{subject to} & q_i(x) \leq 0, & i \in \hat{I}_{in} \\ & q_i(x) = 0, & i \in \hat{I}_{eq} \\ & x \in S. & \end{array}$$

We denote by $\Psi^*(S)$ the dual bound of (QE(S)).

5.2 Assumptions

For constructing locally exact lower bounds we have to assume that a local minimizer of problem (Q) fulfills the following assumption.

Assumption 1
Let x^* be a local minimizer of problem (Q) and $\lambda^* \in I\!R^I$ be the corresponding Lagrange multiplier. The Hessian $\nabla^2 q_0(x)$ is positive semidefinite over $T^+_{x^*}$, i.e.

$$y^T \nabla^2 q_0(x) y \geq 0 \textit{ for all } y \in T^+_{x^*},$$

where the extended tangent space $T^+_{x^*}$ is defined by

$$T^+_{x^*} := \{x \in I\!R^n : \nabla q_i(x^*)^T x = 0 \textit{ for } i \in \mathcal{B}(x^*) \cup I_{eq}\}$$

and

$$\mathcal{B}(x^*) := \{i \in I_{in} : \lambda_i^* > 0\}$$

is the index set corresponding to positive Lagrange multipliers.

We give now several conditions implying Assumption 1.

Lemma 6 *Let x^* be a local minimizer of problem (Q) and $\lambda^* \in I\!R^I$ be the corresponding Lagrange multiplier fulfilling the strict complementarity condition :*

$$\lambda_i^* > 0 \quad \textit{for} \quad i \in \mathcal{A}(x^*)$$

where

$$\mathcal{A}(x^*) := \{i \in I_{in} : q_i(x^*) = 0\}$$

is the index set of active constraints. The following conditions imply Assumption 1:
(i) the point x^* fulfills the modified second order optimality condition: the Hessian $\nabla^2 q_0(x)$ is positive semidefinite over the tangent space T_{x^*} defined by

$$T_{x^*} := \{x \in I\!R^n : \nabla q_i(x^*)^T x = 0 \textit{ for } i \in \mathcal{A}(x^*) \cup I_{eq}\};$$

(ii) the constraints of problem (Q) are linear and x^* fulfills the second order optimality condition: the Hessian $\nabla_x^2 L(x^*, \lambda^*)$ is positive semidefinite over the tangent space T_{x^*};
(iii) the constraints of problem (Q) are linear and x^* is a regular point, i.e. the vectors $\{\nabla q_i(x^*) : i \in \mathcal{A}(x^*) \cup I_{eq}\}$ are linearly independent.

Proof.
(i) From the strict complementarity condition it follows $\mathcal{A}(x^*) = \mathcal{B}(x^*)$. This implies $T^+_{x^*} = T_{x^*}$ which proves the assertion.
(ii) Since the constraints of problem (Q) are linear it holds $\nabla_x^2 L(x, \lambda) = \nabla^2 q_0(x)$. Therefore (ii) is equivalent to (i) in this case.
(iii) Since a local minimizer which is a regular point fulfills the second order optimality condition, (iii) implies (ii).

□

Consider the following example: $\min\{-x^T x : 0 \leq x \leq e\}$, where $x \in I\!R^n$ and $e \in I\!R^n$ is the vector of ones. This problem has a unique global minimizer $x^* = e$ fulfilling the strict complementarity condition. From Lemma 6 (iii) it follows that x^* fulfills Assumption 1.

5.3 The Main Theorem

In this section we present the main Theorem on locally exact dual bounds. We begin with the following result.

Lemma 7 *Let $A \in I\!R^{(n,n)}$ be a symmetric matrix which is is positive semidefinite over the linear subspace span $\{w_1, .., w_p\}^\perp$ where $w_i \in I\!R^n, 1 \le i \le p$. Then there exist $\bar{\alpha} \in I\!R^p$ such that $A + \sum_{i=1}^{p} \alpha_i w_i w_i^T$ is positive semidefinite for all $\alpha \ge \bar{\alpha}$.*

Proof.
Let $B := \sum_{i=1}^{p} \rho_i w_i w_i^T$ where $\rho_i > 0, 1 \le i \le p$. Let $V :=$ span $\{w_1, .., w_p\}$, $R :=$ kern (A), $S := V \cap R^\perp$ and $T := V^\perp \cap R^\perp$. Define

$$c_1 := \min_{x \in T \setminus \{0\}} \frac{x^T A x}{x^T x}, \quad c_2 := \min_{x \in V \setminus \{0\}} \frac{x^T B x}{x^T x}, \quad c_3 := \|A\|_2.$$

Since A is positive semidefinite on $V^\perp$ we have $c_1 > 0$ and using $x^T B x = \sum_{k=1}^{p} \rho_k (w_k^T x)^2 \ge 0$ we infer that the matrix B is positive semidefinite over $I\!R^n$ and positive definite over V implying $c_2 > 0$. Given $x \in I\!R^n$ there exist $r \in R, s \in S$ and $t \in T$ such that $x = r + s + t$ since $I\!R^n = R \bigoplus S \bigoplus T$. Therefore

$$\begin{aligned} x^T (A + \mu B) x &= (s+t)^T A (s+t) + \mu (r+s)^T B (r+s) \\ &\ge c_1 \|t\|^2 - 2c_3 \cdot \|s\| \cdot \|t\| - c_3 \|s\|^2 + \mu \cdot c_2 \cdot (\|r\|^2 + \|s\|^2) \\ &= (\sqrt{c_1}\|t\| - c_2/\sqrt{c_1}\|s\|)^2 + (\mu c_2 - c_3 - c_2^2/c_1)\|s\|^2. \end{aligned}$$

This implies $A + \mu_0 B \succeq 0$ where $\mu_0 = (c_3 + c_2^2/c_1)/c2$. Setting $\bar{\alpha} = \mu_0 \cdot \rho$ we obtain $A + \sum_{i=1}^{p} \alpha_i w_i w_i^T = A + \mu B + \sum_{i=1}^{p} (\alpha_i - \bar{\alpha}_i) w_i w_i^T \succeq 0$.

□

A variant of Lemma 7 is presented in [14] (Debreu's Lemma). We now state the main result.

Theorem 1 *Let x^* be a local minimizer of problem (Q) fulfilling Assumption 1. Given a partition set $S \ni x^*$ define*

$$\delta_i(S) := -\min_{x \in S} \nabla q_i(x^*)^T (x - x^*), \quad i \in \mathcal{B}(x^*). \tag{9}$$

Assume that the constraints of problem (QE(S)) are defined by

$$\begin{aligned} \nabla q_i(x^*)^T (x - x^*)(\nabla q_i(x^*)^T (x - x^*) + \delta_i(S)) \le 0, &\quad i \in \mathcal{B}(x^*) \quad (10) \\ \nabla q_i(x^*)^T (x - x^*) \le 0, &\quad i \in \mathcal{B}(x^*) \quad (11) \\ q_i(x) = 0, &\quad i \in I_{eq} \quad (12) \\ q_i(x)^2 = 0, &\quad i \in I_{eq} \quad (13) \\ q_i(x) \le 0, &\quad i \in \hat{I}_{in} \quad (14) \end{aligned}$$

Then there exist $\delta^* \in I\!R^{\mathcal{B}(x^*)}, \delta^* > 0$, such that

$$\Psi^*(S) = q^*(S) \text{ for all } S \subset S_{\delta^*}$$

where

$$S_{\delta^*} := \{x \in I\!R^n : 0 \ge \nabla q_i(x^*)^T (x - x^*) \ge -\delta_i^*, \quad i \in \mathcal{B}(x^*)\}.$$

Proof. Choose a proper indexing of the constraints of problem (QE) such that $\alpha = (\alpha^{(1)}, \alpha^{(2)}, \alpha^{(3)}, \alpha^{(4)}, \alpha^{(5)})$, where $\alpha^{(1)}, \alpha^{(2)}, \alpha^{(3)}, \alpha^{(4)}$ and $\alpha^{(5)}$ pertain to the constraints (10), (11), (12), (13) and (14) respectively. Assume $\alpha^{(5)} = 0$. Then it holds $L_e(x^*, \alpha) = q_0(x^*)$. From the Karush-Kuhn-Tucker condition

$$\nabla q_0(x^*) + \sum_{i \in \mathcal{B}(x^*) \cup I_{eq}} \lambda_i^* \nabla q_i(x^*) = 0$$

and from

$$\nabla L_e(x^*, \alpha) = \nabla q_0(x^*) + \sum_{i \in \mathcal{B}(x^*)} (\alpha_i^{(1)} \delta_i(S) + \alpha_k^{(2)}) \nabla q_i(x^*) + \sum_{i \in I_{eq}} \alpha_i^{(3)} \nabla q_i(x^*)$$

we obtain

$$\nabla L_e(x^*, \alpha) = \sum_{i \in \mathcal{B}(x^*)} (\alpha_i^{(1)} \delta_i(S) + \alpha_i^{(2)} - \lambda_i^*) \nabla q_i(x^*) + \sum_{i \in I_{eq}} (\alpha_i^{(3)} - \lambda_i^*) \nabla q_i(x^*).$$

From Lemma 7 it follows that there exist $\bar{\alpha}^{(1)} \in I\!R_+^{\mathcal{B}(x^*)}$ and $\bar{\alpha}^{(4)} \in I\!R^{I_{eq}}$ such that $\nabla_x^2 L_e(x^*, \alpha) \succeq 0$ for all $\alpha \in I\!R^{\hat{I}}$ with $\alpha^{(5)} = 0$, $\alpha^{(1)} = \bar{\alpha}^{(1)}$ and $\alpha^{(4)} = \bar{\alpha}^{(4)}$. Choosing $\alpha^{(1)} = \bar{\alpha}^{(1)}$, $\alpha^{(4)} = \bar{\alpha}^{(4)}$, $\alpha_i^{(3)} = \lambda_i^*$ for $i \in I_{eq}$ and $\alpha_i^{(2)} = \lambda_i^* - \bar{\alpha}_i^{(1)} \delta_i(S)$ for $i \in \mathcal{B}(x^*)$ we have $\nabla L_e(x^*, \alpha) = 0$. For $k \in \mathcal{B}(x^*)$ define $\delta_k^* := \lambda_k^* / \bar{\alpha}_k^{(1)}$ if $\bar{\alpha}_k^{(1)} > 0$ and $\delta_k^* := \infty$ if $\bar{\alpha}_k^{(1)} = 0$. For $S \subset S_{\delta^*}$ and $k \in \mathcal{B}(x^*)$ we have $\delta_k(S) \leq \delta_k^*$ implying $\alpha_k^{(2)} = \lambda_k^* - \bar{\alpha}_k^{(1)} \delta_k(S) \geq \lambda_k^* - \bar{\alpha}_k^{(1)} \delta_k^* \geq 0$. Hence (α, x^*) fulfills (7) and by Lemma 5 we conclude that $\Psi^*(S) = q^*(S)$.

□

A consequence of Theorem 1 is that the dual bound $\Psi^*(S)$ is getting exact if the partition set S is diminished sufficiently. As mentioned in the introduction the only known locally exact lower bound for nonconvex smooth optimization problems is the LP-bound of Epperly and Swaney [7].

5.4 Linearly Constrained Problems

In the previous section we used a local minimizer of problem (Q) for constructing a locally exact lower bound. Assuming that the constraints of problem (Q) are linear it is possible to construct locally exact lower bounds without using a local minimizer as a reference point.

Corollary 1 *Assume that the constraints of problem (Q) are linear. Given a partition set S define*

$$\rho_i(S) := - \min_{x \in \Omega \cap S} q_i(x), \quad i \in I_{in}.$$

Assume that the following redundant inequality constraints

$$q_i(x) \cdot (q_i(x) + \rho_i(S)) \leq 0, \quad i \in I_{in} \tag{15}$$

and the following redundant equality constraints

$$q_i(x)^2 = 0, \quad i \in I_{eq}$$

are included in problem (QE(S)). Then $\Psi^*(S)$ is locally exact with respect to all local minimizers of problem (Q) fulfilling Assumption 1.

Proof. Since the constraints (10)-(14) are included in problem (QE(S)) for all local minimizers x^* of problem (Q) the assertion follows from Theorem 1.

$\square$

If the number of constraints of problem (Q) is not too large the computational cost for solving problem (QE) as defined in Corollary 1 is still reasonable. This applies for example for the box-constrained quadratic program and the standard quadratic program which we will consider in the sequel. The box-constrained quadratic program is defined by

$$\text{(BQ)} \qquad \begin{array}{rl} \text{global minimize} & q_0(x) \\ \text{subject to} & \underline{x} \le x \le \bar{x}, \end{array}$$

where $\underline{x}, \bar{x} \in I\!R^n$. Using the redundant constraints (15) we obtain the following extended box-constrained quadratic program:

$$\text{(BQE)} \qquad \begin{array}{rl} \text{global minimize} & q_0(x) \\ \text{subject to} & \underline{x} \le x \le \bar{x}, \\ & (x_i - \underline{x}_i)(x_i - \bar{x}_i) \le 0, \quad 1 \le i \le n. \end{array}$$

From Corollary 1 it follows that the dual bound of problem (BQE), denoted by Ψ^*_{bqe}, is locally exact with respect to all minimizers of problem (BQ) fulfilling Assumption 1. Denote by $L_{bqe}(x, \alpha)$ the Lagrangian of problem (BQE). Note that the lower bound used in the global optimization method α-BB ([1]) is obtained by choosing a specific value α such that $\nabla^2_x L_{bqe}(x, \alpha) \succ 0$. From this it follows that in general Ψ^*_{bqe} is more accurate than the α-BB bound. Another important quadratic program is the standard quadratic program defined by

$$\text{(SQ)} \qquad \begin{array}{rl} \text{global minimize} & q_0(x) \\ \text{subject to} & 0 \le x \le e, \\ & e^T x - 1 = 0, \end{array}$$

where $e \in I\!R^n$ is the vector of ones. Using the redundant constraints of Corollary 1 we obtain

$$\text{(SQE1)} \qquad \begin{array}{rl} \text{global minimize} & q_0(x) \\ \text{subject to} & 0 \le x \le e, \\ & x_i(x_i - 1) \le 0, \quad 1 \le i \le n \\ & e^T x - 1 = 0, \\ & (e^T x - 1)^2 = 0. \end{array}$$

Similarly as above it follows that the dual bound of problem (SQE1) is locally exact with respect to all minimizers of problem (SQ) fulfilling Assumption 1. A different extended quadratic program for problem (SQ) is

$$\text{(SQE2)} \qquad \begin{array}{rll} \text{global minimize} & q_0(x) & \\ \text{subject to} & x \ge 0, & \\ & x_i x_j \ge 0, \quad ij \in E_c & (16) \\ & e^T x - 1 = 0, & \\ & (e^T x - 1)^2 = 0 & \end{array}$$

where $E_c := \{ij : 1 \le i < j \le n, \partial_{ii} q_0(x) - 2\partial_{ij} q_0(x) + \partial_{jj} q_0(x) > 0\}$. Denote by Ψ^*_{sqe1} and by Ψ^*_{sqe2} the dual bounds of (SQE1) and (SQE2) respectively.

Proposition 3
(i) The dual bound Ψ^*_{sqe2} *is locally exact with respect to all minimizers of (SQ) fulfilling Assumption 1.*
(ii) It holds $\Psi^*_{sqe1} \le \Psi^*_{sqe2}$.

Proof. Denote by $L_1(x,\alpha)$ and $L_2(x,\alpha)$ the Lagrange functions of (SQE1) and (SQE2) respectively and let $(\hat{x},\alpha^*)$ be such that $L_1(\hat{x},\alpha^*) = \Psi^*_{sqe1}$. From [17] it follows that the constraints (16) can be replaced by the constraints

$$x_i x_j \ge 0, \quad 1 \le i,j \le n.$$

Let $x \in I\!R^n$ be a point fulfilling $e^T x - 1 = 0$. Then

$$x_i(x_i - 1) = - \sum_{1 \le k \le n, k \ne i} x_i x_k, \quad 1 \le i \le n+1.$$

This implies that there exist $\hat{\alpha}$ such that $L_1(x,\alpha^*) = L_2(x,\hat{\alpha})$ for all $x \in I\!R^n$ with $e^T x = 1$. From Lemma 2 it follows

$$\Psi^*_{sqe1} = \min_{e^T x = 1} L_1(x,\alpha^*) = \min_{e^T x = 1} L_2(x,\hat{\alpha}) \le \Psi^*_{sqe2}.$$

This proves the assertion.

□

6 Optimality Cuts

Based on Theorem 1 we can construct a cutting plane cutting off a given local minimizer from the feasible set. A consequence of Theorem 1 is:

Corollary 2 *Let* x^* *be a local minimizer of problem (Q) fulfilling Assumption 1 and let* $H \subset I\!R^n$ *be a half-space such that* $x^* \in \text{ int } H$ *and* $\Omega \cap H \subset S_{\delta^*}$. *Then* $q^*(H) = q_0(x^*)$, *where* S_{δ^*} *is defined as in Theorem 1.*

A halfspace which meets the conditions of Corollary 2 defines an optimality cut with respect to x^*, i.e. H cuts off x^* from the feasible set. The following Lemma gives a recept for constructing H.

Proposition 4 *Let* x^* *be a local minimizer of problem (Q) fulfilling Assumption 1. Define the matrix*

$$A(\alpha) := \nabla^2 q_0(x^*) + \sum_{i \in \mathcal{B}(x^*) \cup I_{eq}} \alpha_i w_i w_i^T,$$

where $w_i := \nabla q_i(x^*)$. *Let* $\hat{\alpha} \in I\!R^{\mathcal{B}(x^*) \cup I_{eq}}$ *be a parameter fulfilling* $A(\hat{\alpha}) \succeq 0$ *and* $\hat{\alpha}_i \ge 0$ *for* $i \in \mathcal{B}(x^*)$ *(which exists according to Lemma 7). Let* $\eta := \sum_{i \in \mathcal{B}(x^*)} -\frac{\hat{\alpha}_i}{\lambda_i^*} w_i$ *where* λ_i^* *are the Lagrange parameters corresponding to* x^*. *Then*

$$H = \{x \in I\!R^n : \eta^T (x - x^*) \le 1\}$$

defines an optimality cut with respect to x^*.

Proof. Obviously, it holds $x^* \in \text{ int } H$. Let K_{x^*} be the cone defined by

$$K_{x^*} := \{x \in I\!R^n : w_i^T(x - x^*) \leq 0 \text{ for } i \in \mathcal{B}(x^*)\}.$$

Let

$$V_j = \{x \in I\!R^n : w_j^T(x - x^*) = -\delta_j^*, w_i^T(x - x^*) = 0, i \in \mathcal{B}(x^*) \setminus \{j\}\}$$

for $j \in \mathcal{B}(x^*)$ and

$$V_0 = \{x \in I\!R^n : w_i^T(x - x^*) = 0, i \in \mathcal{B}(x^*)\}$$

where $\delta_i^* = \frac{\lambda_i^*}{\hat{\alpha}_i}$ if $\hat{\alpha}_i > 0$ and $\delta_i^* = \infty$ else. It holds $\eta^T(x - x^*) = \delta_i^*$ for $x \in V_i$ and $i \in \mathcal{B}(x^*)$ and $\eta^T(x - x^*) = 0$ for $x \in V_0$. Hence $H \cap K_{x^*} = \text{ conv } \{V_i : i \in \mathcal{B}(x^*) \cup \{0\}\}$ and due to $V_i \subset S_{\delta^*}$ for $i \in \mathcal{B}(x^*) \cup \{0\}$ we have

$$H \cap \Omega \subset H \cap K_{x^*} \subset S_{\delta^*}.$$

From the proof of Theorem 1 it follows that $q^*(S_{\delta^*}) = q_0(x^*)$. Using Corollary 2 this proves the assertion.

□

The parameter $\hat{\alpha}$ should be computed such that $\text{ diam } (S_{\delta^*})$ is as large as possible. Since $\delta_i^*/|w_i|$ is an upper bound on the diameter of S_{δ^*} along the direction w_i this is similar to maximize $\delta_i^*/|w_i|$ for all $i \in \mathcal{B}(x^*)$ or to minimize $\sum_{i \in \mathcal{B}(x^*)} \frac{1}{\delta_i^*}|w_i| = \sum_{i \in \mathcal{B}(x^*)} \frac{\hat{\alpha}_i}{\lambda_i^*}|w_i|$. This motivates to compute $\hat{\alpha}$ by the following semidefinite program:

$$\begin{aligned} \hat{\alpha} = \ \text{argmin} \quad & \sum_{i \in \mathcal{B}(x^*)} \frac{\alpha_i}{\lambda_i^*}|w_i| \\ s.t. \quad & A(\alpha) \succeq 0 \\ & \alpha_i \geq 0, \quad i \in B(x^*). \end{aligned} \tag{17}$$

From Theorem 1 it follows that $\hat{\alpha}$ is well-defined if x^* fulfills Assumption 1. Note that for the construction of an optimality cut it is sufficient to find a feasible point of (17) which is a much simpler problem than solving (17).

7 Conclusion

We presented locally exact lower bounds and optimality cuts for problem (Q). If all global minimizers of problem (Q) fulfill Assumption 1 then an appropriate B&B algorithm using either locally exact lower bounds or optimality cuts terminates in finite time. Approaches how these result can be applied to twice-differentiable global optimization problems were presented in [16]. We are currently implementing the lower bounding technique and the method for obtaining optimality cuts in a B&B algorithm. Numerical results will be published in a subsequent paper.

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